

широкая полоса Fe^{3+} при $\lambda \approx 725$ нм на оптическом переходе ${}^4\text{T}_1(\text{G}) \rightarrow {}^6\text{A}_1(\text{S})$. Причем, с увеличением содержания железа в образцах интенсивность этой полосы резко снижается вплоть до нуля при 5,0 масс.% Fe_2O_3 . В некоторых образцах второй серии на коротковолновом крыле этой полосы появляются R-линии Cr^{3+} в кианите (Al_2SiO_5). В спектре ИКЛ ряда образцов этой серии, спеченных в вакууме при температуре 1300 °С в течении 1 часа, появляется дополнительная широкая слабая полоса при $\lambda \approx 525$ нм. Обсуждаются результаты исследований.

1. Wickersheim K. A., Lefever R. A., J. Opt. Soc. Am., 50, 831-832 (1960).

THE MAGNETIC ANISOTROPY OF SPIN $S=1$ BaMoP_2O_8 SYSTEM

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In this work the magnetic anisotropy of low dimensional magnetic compound BaMoP_2O_8 was studied by using density functional theory and inelastic neutron scattering techniques. Obtained results show that anisotropy of the system has the easy-axis character, where the on-site term plays the leading role in stabilisation of the magnetic ordering.

The magnetic anisotropy, originated from spin-orbit coupling effects, is considered to be the one of the main characteristic, which stabilises the magnetic ordering of the system. It may contain the intersite symmetric and antisymmetric terms known as Dzyaloshinskii-Moriya interaction (DMI), arising due to lack of inversion symmetry [1], and on-site anisotropy, which takes place only for situations, when spin S of magnetic atoms is more than 1/2. From the theoretical side, corresponding values of anisotropic characteristics can be investigated on the level of density functional theory (DFT), while in the experiment it is required to use more sophisticated techniques. The inelastic neutron scattering (INS) is considered to be the powerful method, which is able not only to give the value of magnetic interactions quantitatively, but also can identify the individual components of on-site and intersite anisotropy of the system.

The low dimensional magnetic compound BaMoP_2O_8 contains the triangular regular lattice of molybdenum atoms. Recently, it was revealed by neutron diffraction experiment that the system follows to stripe antiferromagnetic order with propagation vector $\mathbf{k} = (1/2, 1/2, 1/2)$. Theoretically, it was shown that the magnetic model is highly frustrated and has one dimensional character [2]. Further calculations of anisotropic energies, taking the correlations through on-site Coulomb parameter U and spin-orbit

coupling effects on the level of perturbation theory, demonstrate that magnetic moments of molybdenum atom should be oriented along easy axis, which corresponds to anisotropic energy minimum. Utilisation of INS revealed the clear magnetic excitations at 20 meV, and fitting of them also gives the easy axis, where anisotropic terms are in reasonable agreement with theory (Fig.1).

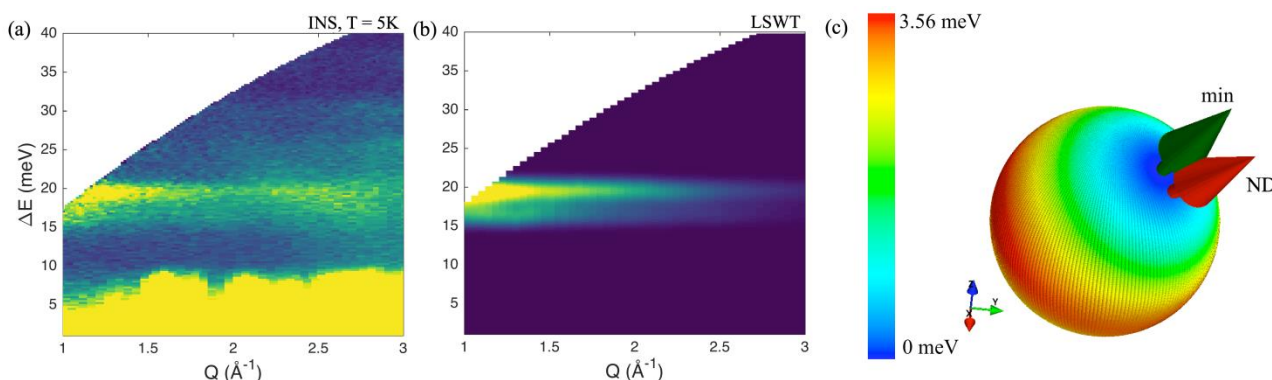


Fig. 1. (a) Inelastic neutron scattering spectra obtained for powder sample of BaMoP₂O₈. (b) The fitted spectra by using anisotropic spin model. (c) The 3D map of anisotropic energy, obtained on the level of DFT+U method. The green arrow denoted as «min» corresponds to minimum of anisotropic energy, while the red arrow «ND» — easy axis from neutron experiment.

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1. Moriya T. et al., Phys. Rev. 120, 91 (1960).
2. Hembacher J. et al., Phys. Rev. B 98, 094406 (2018).

STRUCTURE OF CDTE NANOCRYSTALS SYNTHESIZED BY ELECTROCHEMICAL DEPOSITION FROM DIFFERENT SOLUTIONS ONTO THE SiO₂/SI TRACK TEMPLATE

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The main aim of this study is CdTe nanocrystals growing by electrochemical deposition in the a-SiO₂/Si -n track template.

CdTe is a direct bandgap semiconductor group A^{II}B^{VI} with $E_g=1.49$ eV at 300 K [1]. It is known that CdTe is one of the materials most suitable for solar cells production [2]. Nanocrystals, such as CdSe, ZnS, ZnSe, CdS and PbS, have nonlinear optical susceptibility, which makes it possible to use them as materials for passive optical shutters for the generation of ultrashort laser pulses in the near-IR range [3, 4].